# Interaction between an insulating material and a plasma. A molecular dynamic simulation approach.

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# INTERACTION BETWEEN AN INSULATING MATERIAL AND A PLASMA. A MOLECULAR DYNAMICS SIMULATION APPROACH

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## ABSTRACT

In this paper, we present the results of the simulation of the interaction between incident particles and a polyethylene area. The particles can be the $SF_6$ molecules or the copper ions ionized once. We report the evolution versus time of various parameters like the temperature or the energy of the polyethylene crystal for several initial velocities of the incident particles. The velocities can be $V_i$ = 3, 5, 7 or 9 km.s$^{-1}$, that corresponds to a particle with an average energy of 2.94 eV to 61.3 eV. We discuss the efficiency of the energy transfer between the energetic particles and the polymer. For this, a distinction is made in the assessment of intra and inter-molecular forces for giving an explanation of a possible change in the molecular structure of the polyethylene crystal. Finally, the radius of gyration of the polymer has been calculated. It is shown that, the biggest average initial speeds of the incident particles are needed to speak of a hypothetical local change of state of the polymer.

## 1. INTRODUCTION

The survey of plasmas and their numerous applications is more and more important in the domain of the fundamental research. In the field of the protection of electrical networks, the technological screw is located in the control of the interaction between the plasma and its surrounding material. Indeed, the damages induced to the material by the plasma could seriously reduce the life span of the electrical devices. It is really necessary to understand what happen, and especially knowing the major physical phenomena that we must take into account. In several industrial applications, the plasma interacts with an insulating material. During the interaction, the deterioration of the polymer is accompanied by a significant loss of matter as named ablation.

Instead of studying this interaction at the macroscopic scale, we propose to do a study at the microscopic scale or more precisely at the atomic level. For this, we use molecular dynamic simulations. Therefore, a molecular model of a common polymer has been developed to study and to understand the ablation mechanism when a plasma interacts with an insulating wall. The chosen polymer is the polyethylene $(CH_2)_n$ due to its simple molecular scheme, the macromolecule is plane and linear. From this model, the transfer of energy between incident particles and the polymer area can be valued and the material ablation is considered as a local molecular destruction of the macromolecule, bond breaking...

## 2. MODEL DESCRIPTION

### 2.1 Polyethylene model

The total energy of the polyethylene crystal is described with several potentials. We distinguish the intra-molecular and inter-molecular potentials as the atoms are bonded or not. The bonded potentials named $V_2$, $V_3$ and $V_4$ are used to describe, respectively, the interaction between two, three and four bonded atoms. The interactions between non-bonded atoms are treated as Van Der Waals ($V_{vdw}$) and electrostatic ($V_{elec}$) interactions. So, the potential energy of the polyethylene crystal could be written as:

$$V = V_2 + V_3 + V_4 + V_{vdw} + V_{elec} \qquad (1)$$

To describe the polyethylene covalent bond (C-C and C-H bonds), we use a Morse potential [1,2]. This potential is given in the Eq. 2, where $r_{ij}$ is the inter-nuclear separation distance between atom $i$ and $j$, $R_e$ is the equilibrium distance between the two atoms. $D$ and $\gamma$ are given in Table 1.

$$V_2(r_{ij}) = D\left[1 - \exp\left(-\gamma\left(r_{ij} - R_e\right)\right)\right]^2 \qquad (2)$$

The bending angle between three consecutive bonded atoms is described by a cosine function and is given in Eq. 3, where $\theta_{ijk}$ is the angle formed by three consecutive bonded atoms, $K$ and $\theta_0$ are given in Table 1.

$$V_3(\theta_{ijk}) = SW(r_{ij})SW(r_{jk}) \cdots \times \frac{K}{2}\left[\cos(\theta_{ijk}) - \cos(\theta_0)\right]^2 \quad (3)$$

$SW(\mathrm{r})$ are the switching function between two bonded atoms. The $V_4$ potential describe the torsional interaction between four consecutive bonded atoms. This potential is given in Eq. (4), its internal parameter is the dihedral angle $\tau_{ijkl}$. The constant parameters $A$ and $B$ are given in Table 1.

$$V_4(\tau_{ijkl}) = SW(r_{ij})SW(r_{jk})SW(r_{kl}) \cdots \times SW(\theta_{ijk})SW(\theta_{jkl}) \cdots \times \left[-A\cos(\tau_{ijkl}) + B\cos^3(\tau_{ijkl})\right] \quad (4)$$

$SW(\Theta)$ are the bending switching functions between three bonded atoms. These functions are used to add to the model the possibility to simulate the bond breaking. Indeed, the switching functions attenuate the bending and the torsional potentials when the local bond is extremely long and ultimately broken. We consider that a bond is broken, if the distance between two consecutive atoms is greater than 0.4 nm [5].

To define $SW(\mathrm{r})$, we use the trigonometric function given by [4,6]:

$$SW(\mathrm{r}) = 1 - \tanh\left[1.53131681.10^{-7}(\mathrm{r} - R_e) \cdots \times (\mathrm{r} + 4.669625)^8\right] \quad (5)$$

where $\mathrm{r}$ refers to $r_{ij}$, $r_{jk}$ or $r_{kl}$ distances between two bonded atoms. Of the point of mathematical view, the derivative of the torsional potential is proportional to $\sin\theta^{-1}$, and when the angle is close to π we get a mathematical singularity. To avoid this problem we must add bending switching functions to the torsional potential to keep the stability of the model. This function is given by [4,6]:

$$SW(\Theta) = \left(1 - \cos^{16}\Theta\right)^4 \quad (6)$$

where $\Theta$ refers to $\theta_{ijk}$ or $\theta_{jkl}$ angles between three bonded atoms.

For describing the interaction between the atoms that are in different polymer chains or the interaction between the atoms that are in the same chains but are arranged to more of four consecutive bonds, we use the conventional Lennard-Jones and electrostatic potentials. The Lennard-Jones potential is given in Eq. (7), where $\varepsilon_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ represent, respectively, the energy parameter and the core diameter of the interaction between atom type $\alpha$ and atom type $\beta$. These constant parameters are given in Table 1. $r_{\alpha\beta}$ is the distance between the two non bonded atoms.

$$V_{vdw}(r_{\alpha\beta}) = 4\varepsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r_{\alpha\beta}}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r_{\alpha\beta}}\right)^{6}\right] \quad (7)$$

Table 1. Polyethylene potential parameters [3,4]

| Potential | Interaction type | Parameters |
|---|---|---|
| $V_2(r_{ij})$ | C-C | $D_{CC} = 334.944\ kJ.mol^{-1}$ |
| | | $R_{eCC} = 0.153\ nm$ |
| | | $\gamma_{CC} = 19.4\ nm^{-1}$ |
| | C-H | $D_{CH} = 446.732\ kJ.mol^{-1}$ |
| | | $R_{eCH} = 0.109\ nm$ |
| | | $\gamma_{CH} = 17.5\ nm^{-1}$ |
| $V_3(\theta_{ijk})$ | C-C-C | $K_{CCC} = 130.220\ kJ.mol^{-1}$ |
| | | $\theta_{0CCC} = 1.9549433\ rad$ |
| | C-C-H | $K_{CCH} = 75.380\ kJ.mol^{-1}$ |
| | | $\theta_{0CCH} = 1.9006636\ rad$ |
| | H-C-H | $K_{HCH} = 70.060\ kJ.mol^{-1}$ |
| | | $\theta_{0HCH} = 1.9074703\ rad$ |
| $V_4(\tau_{ijkl})$ | C-C-C-C | $A = 18.422\ kJ.mol^{-1}$ |
| | | $B = 26.796\ kJ.mol^{-1}$ |
| $V_{vdw}(r_{ij})$ | C…C | $\varepsilon_{CC} = 0.4257\ kJ.mol^{-1}$ |
| | | $\sigma_{CC} = 0.335\ nm$ |
| | H…H | $\varepsilon_{HH} = 0.07151\ kJ.mol^{-1}$ |
| | | $\sigma_{HH} = 0.281\ nm$ |
| | C…H | $\varepsilon_{CH} = 0.1745\ kJ.mol^{-1}$ |
| | | $\sigma_{CH} = 0.308\ nm$ |
| $V_{elec}(r_{ij})$ | | $q_C = -0.2\ q_e$ |
| | | $q_H = +0.1\ q_e$ |

The Lennard Jones parameters for non pure mixtures are computed from the Lorentz-Berthelot mixing rules given in Eq. (8):

$$\varepsilon_{\alpha\beta} = \left(\varepsilon_{\alpha\alpha}\varepsilon_{\beta\beta}\right)^{\frac{1}{2}},\ \sigma_{\alpha\beta} = \frac{1}{2}\left(\sigma_{\alpha\alpha} + \sigma_{\beta\beta}\right) \quad (8)$$

The electrostatic potential is given in Eq. (9), where $q_\alpha$ and $q_\beta$ represent the partial charges in electron charge units of atom type $\alpha$ and atom type $\beta$, these constant parameters are given in Table 1 and are taken from [7]. $\varepsilon_0$ is the vacuum permittivity and $r_{\alpha\beta}$ is the distance between the two non bonded atoms.

$$V_{coul}(r_{\alpha\beta}) = \frac{1}{4\pi\varepsilon_0}\frac{q_\alpha q_\beta}{r_{\alpha\beta}} \qquad (9)$$

### 2.2 Polyethylene structure

The polyethylene crystal is in the orthorhombic phase and the unit cell lengths along the *a*, *b* and *c* axis are the same than those defined in the Cartesian coordinates *x*, *y* and *z*. The cell parameters are *a = 0.74 nm*, *b = 0.49 nm* and *c = 0.26 nm*. The polyethylene crystal is made of 61 chains of 75 carbon atoms and therefore of 150 hydrogen atoms, what corresponds to a total number of 13 725 atoms. The polymer dimensions are 4.5, 3.0 and 9.5 nm along *x*, *y* and *z* axis, respectively. A polyethylene crystal view is given in Figure 1.

Concerning the initial conditions, the coordinate of the atoms and their conjugated momenta must be chose correctly. Firstly, the distance between two consecutive atoms and the angle formed by three and four consecutive bonded atoms have been set to minimize all intra-molecular potentials $V_2$, $V_3$ and $V_4$, respectively. Thus for each possible interaction, all the polymer atoms are placed to their equilibrium position. Secondly, the conjugated momenta are chosen from a Gaussian distribution in the range of ± $V_{max}$. The convergence criterion is that the velocity of the polymer center of mass is equal to zero.

$$\sum_{i=1}^{N_C}\frac{p_i^2}{2M_C} + \sum_{j=1}^{N_H}\frac{p_j^2}{2M_H} = \frac{3}{2}N_T k_B T \qquad (10)$$

where $N_T$ is the total number of atoms in the crystal, $N_C$ and $N_H$ are the total number of carbon and hydrogen atoms, respectively, $k_B$ is Boltzmann's constant, and $T$ is the temperature. $p_i$ and $p_j$ are the atomic momenta of carbon and hydrogen atoms, respectively.

### 2.3 $SF_6$ molecule and copper ion model

The interaction between the copper ion and the other atoms is described with the Lennard-Jones 12-6 potential. For the copper-copper non bonded interactions, the Lennard-Jones potential parameters are taken from [8,9]. As this particle is ionised, we apply the electrostatic potential and this one is used as well as this incident particle interacts inside the polyethylene crystal. The corresponding potential parameters are given in Table 2.

The initial velocities of the incident particles are assigned from a Gaussian distribution between ±*Vi*. The impact angle is defined like being the angle between the incident particle trajectory and the target wall and it is randomly drawn in the range of 30° to 90°. We have chosen these angle values because in our previous works [12], we have shown that for an angle lower to 30° the interaction is sufficiently strong to induce the local polymer destruction, what is not the goal of this work. In order to get a better efficiency, in terms of energy dissipation or polymer's local disorder survey, the incident particles impact the polymer in the middle of its exposed area. Approximately, an incident particle impacts the polymer surface all two picoseconds.

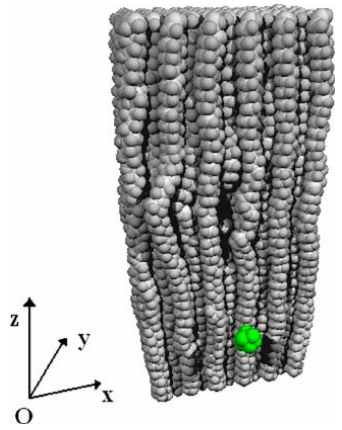


Fig. 1. Polyethylene crystal view: the average incident particles velocities are Vi = 9 km.s$^{-1}$

### 2.4 Equations of motion

The integration of the equations of motion is carried out using an explicit Runge-Kutta-Nyström method with a symplectic integrator [13,14]. The equations of motion, called Hamilton's equations, are given by:

$$\frac{\partial p_i}{\partial t} = \dot{p}_i = -\frac{\partial H}{\partial r_i}, \frac{\partial r_i}{\partial t} = \dot{r}_i = \frac{\partial H}{\partial p_i} \qquad (11)$$

where $r_i$ and $p_i$ are canonically conjugated coordinates and momenta, respectively. The Hamiltonian of the system is given by:

$$H_T = H_{PE} + H_{Cu+} + H_{SF6} \qquad (12)$$

Table 2. Potential parameters for the $SF_6$ molecule and the copper ion particles

| Potential | Interaction type | Parameters |
|---|---|---|
| $V_2(r_{ij})$ | S-F | $D_{SF} = 318.399\ kJ.mol^{-1}$ |
| | | $R_{eSF} = 0.1597\ nm$ |
| | | $\gamma_{SF} = 21.4\ nm^{-1}$ |
| $V_3(\theta_{ijk})$ | F-S-F | $K_{FSF} = 78.530\ kJ.mol^{-1}$ |
| | | $\theta_{0orthoFSF} = 1{,}5707963\ rad$ |
| | | $\theta_{0alignFSF} = 3{,}1415926\ rad$ |
| $V_{vdw}(r_{ij})$ | Cu…Cu | $\varepsilon_{CuCu} = 39.4914\ kJ.mol^{-1}$ |
| | | $\sigma_{CuCu} = 0.2377\ nm$ |
| | Cu…C | $\varepsilon_{CuC} = 4.1002\ kJ.mol^{-1}$ |
| | | $\sigma_{CuC} = 0.285\ nm$ |
| | Cu…H | $\varepsilon_{CuH} = 1.6805\ kJ.mol^{-1}$ |
| | | $\sigma_{CuH} = 0.258\ nm$ |
| | Cu…S | $\varepsilon_{CuS} = 7.7518\ kJ.mol^{-1}$ |
| | | $\sigma_{CuS} = 0.293\ nm$ |
| | Cu…F | $\varepsilon_{CuF} = 4.1637\ kJ.mol^{-1}$ |
| | | $\sigma_{CuF} = 0.259\ nm$ |
| | S…S | $\varepsilon_{SS} = 1.5216\ kJ.mol^{-1}$ |
| | | $\sigma_{SS} = 0.352\ nm$ |
| | S…F | $\varepsilon_{SF} = 0.8173\ kJ.mol^{-1}$ |
| | | $\sigma_{SF} = 0.318\ nm$ |
| | F…F | $\varepsilon_{FF} = 0.4390\ kJ.mol^{-1}$ |
| | | $\sigma_{FF} = 0.283\ nm$ |
| | S…C | $\varepsilon_{SC} = 0.8048\ kJ.mol^{-1}$ |
| | | $\sigma_{SC} = 0.344\ nm$ |
| | S…H | $\varepsilon_{SH} = 0.3299\ kJ.mol^{-1}$ |
| | | $\sigma_{SH} = 0.317\ nm$ |
| | F…C | $\varepsilon_{FC} = 0.4323\ kJ.mol^{-1}$ |
| | | $\sigma_{FC} = 0.309\ nm$ |
| | F…H | $\varepsilon_{FH} = 0.1772\ kJ.mol^{-1}$ |
| | | $\sigma_{FH} = 0.282\ nm$ |
| $V_{elec}(r_{ij})$ | | $q_{Cu} = +1.0\ q_e$ |
| | | $q_S = +0.6\ q_e$ |
| | | $q_F = -0.1\ q_e$ |

The equations of motions are integrated using a timestep of 1 fs. The simulation is composed of two parts. The first one corresponds to an equilibrium phase, of a duration of 10 ps. Indeed, this is the time necessary to the model to reach its equilibrium state from the initial conditions. The second one, of a duration of 30 ps, is the production phase to study the interaction between the incident particles and the polymer. Therefore the total simulation time is 40 ps. The inter-molecular interactions have been computed using a cut-off $r_c$ of 1.2 nm. The simulation has been performed in the micro canonical constant-NVE ensemble.

## 3. RESULTS AND DISCUSSION

### 3.1 Model equilibration

At $t = 0$, the total energy of the polymer is purely kinetic due to our choice of the initial conditions. Thereafter, this energy is redistributed between the potential and the kinetic part of the Hamiltonian. It is shown in Figure 2.a that the system needs approximately 5 ps to reach its equilibrium state. From this configuration, the temperature of the crystal is computed from 5 to 10 ps, and we get an average value of 294.1 ± 1.5 K. In the same time, we have calculated the average value of the total energy of the system that is about 71 565 ± 200 $kJ.mol^{-1}$. With a variation of temperature lower to 1% and a variation of energy of about 0.3%, we can say that the total energy of the system is conserved and that our model is numerically steady.

In the next stage, we would like to verify if a slow energy deposition would be able to induce a meaningful disorder of the molecular structure of the polymer. For this, six particles, two $SF_6$ molecules and four ions of copper, will interact with the polyethylene with several initial velocities. The average speed of the particles will be successively of 3, 5, 7 and 9 $km.s^{-1}$, the corresponding energy of the particles in electron-volt (eV) are given in Table 3. These energies are calculated from the average kinetic energy of particles in a gas. For each simulation, we report several physical parameters, like the temperature or the energy of the crystal but also the autocorrelation functions of the radius of gyration, of the velocity...

Table 3. Average energy (eV) of the incident particles

| $V_i$ ($km.s^{-1}$) | 3 | 5 | 7 | 9 |
|---|---|---|---|---|
| $Cu^+$ | 2.94 | 8.16 | 16.0 | 26.4 |
| $SF_6$ | 6.81 | 18.9 | 37.1 | 61.3 |

### 3.2 Temperature and energy variations of the polyethylene crystal

The temperature, as a function of time, of the polyethylene crystal for the initial velocities of the particles of 3, 5, 7 and 9 $km.s^{-1}$ are given in Figure 2.b and 2.c, respectively. For the lower case, the interaction is not very important and the crystal reaches very quickly an equilibrium state with an average temperature of 296.5 ± 1.6 K. The incident particles haven't got enough kinetic energy to vanquish the

surface's energy of the polymer and to impact it. We can only observe a slight rise of temperature of about 2 K.

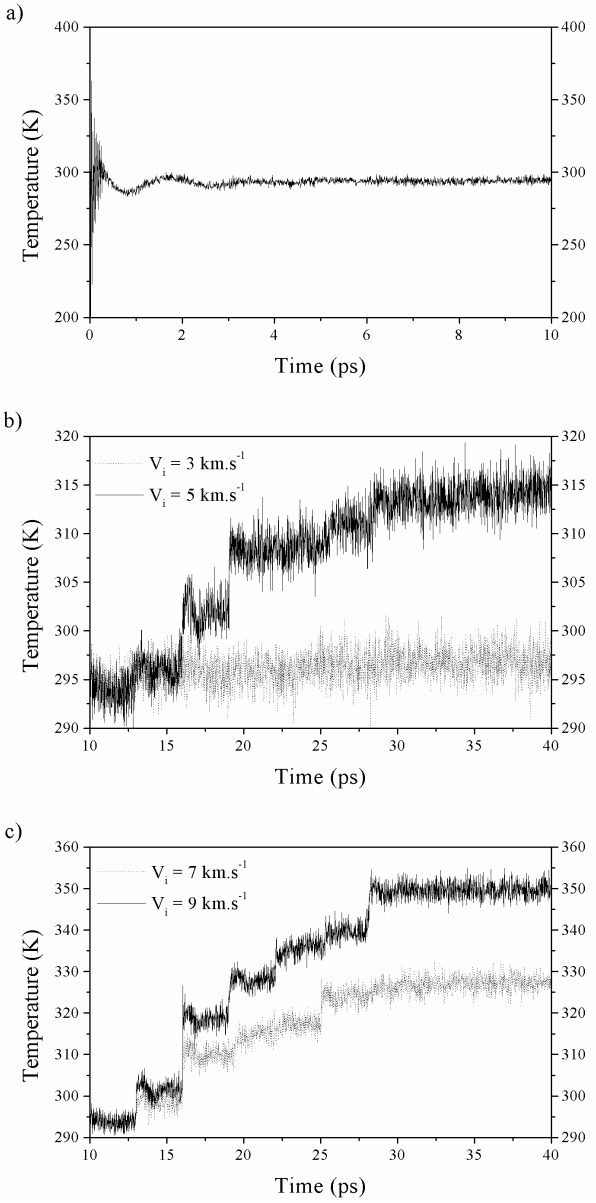


Fig. 2. Polyethylene crystal temperature versus time. a) Equilibration phase. b) Interaction phase: the average incident particles velocities are $V_i$ = 3 and 5 km.s$^{-1}$. c) Interaction phase: the average incident particles velocities are $V_i$ = 7 and 9 km.s$^{-1}$.

In the other cases, the rise of temperature is more sensitive. The new equilibrium temperature of the crystal, that is computed after the interaction, from 30 to 40 ps, is of 313, 9 ± 1.7 K for the average initial velocities of 5 km.s$^{-1}$, that corresponds at an increase of temperature of 20 K. For the average velocities of 7 and 9 km.s$^{-1}$, the crystal temperature rises of 33 K and 56 K, respectively. It is obvious that for the biggest speed, the equilibrium temperature of the crystal of polyethylene is the more important, but it is interesting to see that when an incident particle left its energy to the polymer, it induces a little or a big jump of temperature as it is energetic or not. In a previous work [12], we have shown that the incident particles, which interact with the polymer area, lose all their kinetic energy, and can be trapped inside the polymer. The depth of the interaction is directly proportional to the kinetic energy of the particle. But now, we want to know how this energy is distributed inside the molecular structure of the polyethylene crystal. What are the consequences about the conformational changes of the macromolecule?

Figure 3.a and 3.b show the variations of the kinetic, the intra and inter-molecular energies of the polyethylene crystal versus time, for the average velocities of the incident particles of 3 and 9 km.s$^{-1}$, respectively. Concerning the Figure 3.b, we must specify that for the two other velocities, 5 km.s$^{-1}$ and 7 km.s$^{-1}$, the curves follow the same tendencies. This is the reason for which we do not show them. The variation of the energy is expressed in percentages. Figure 3.a confirms, in this case, that the interaction is weak, and that the variation of the three kind of energy is lower to 5 %. On the other hand, a difference between the three different energies is shown in Figure 3.b. The kinetic and the intra-molecular energies vary of 20% and 105%, respectively, whereas, the inter-molecular energy display a variation of only 5%. First of all, the collision between the incident particles and the polyethylene atoms lead to a bigger molecular agitation due to the increase of the polymer's kinetic energy. This increase is not sufficient to reach the melting temperature of the polymer that is of 410 K, indeed in the case where the initials velocities are the biggest the equilibrium temperature of the crystal is only of 350 K. After, in Figure 3.b it is clearly exposed that a great part of the energy of the incident particles is directly transmitted to the intra-molecular part of the polymer energy. This increase of 105% must be divided between the three intra-molecular forces: the covalent bond ($V_2$), the bending angle ($V_3$) and the dihedral angle ($V_4$). Figure 4 represents evolution of these intra-molecular potentials versus time for the average velocities of the incident particles of 9 km.s$^{-1}$. From this figure, we can see that the energy is not proportionately redistributed between the three intra-molecular potentials. The energy corresponding of the bending angle between three consecutive bonded atoms increase of 66% whereas the energy corresponding of the Morse potential and the energy describing the torsional interaction between four consecutive bonded atoms increase of only 25% and 16%, respectively. The bending potential is used to simulate the elasticity of a polymer chain, in other words if the molecule can be stretched or not. In our model, we have fixed in space the extremities of the polymer chains; therefore this result is not surprising. As the polyethylene crystal is constrained between two parallel plans (xOy), Figure 1, the forces applied in the longitudinal direction of the

macromolecule are the more important. It is more difficult to distort the polymer in the Oz direction than in the two others. The Morse potential, that is used to model the covalent bond, has a little variation and seems to be less sensitive of the interaction, indeed we do not observe any bond breaking all along the simulation time. The $V_4$ potential is used to simulate the fact that the backbone of a polymer chain is in only one plan. But, it can also be used to say if the polymer changes its molecular state, or if the conformational disorder of the molecule is important [15,16]. Due to the small energy variation seen in Figure 4, and due to the small temperature variation shown in Figure 2.c, we can conclude that there are not changes of state of the polymer crystal.

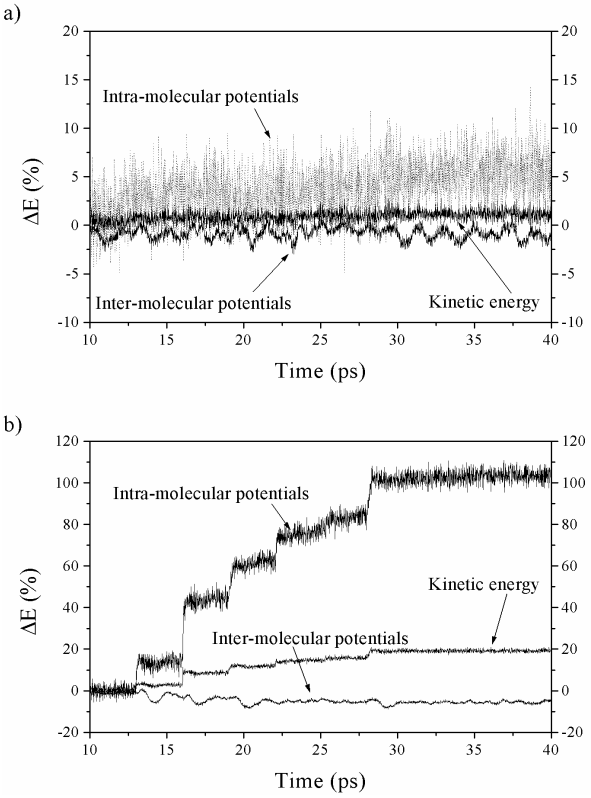


Fig. 3. Polyethylene crystal intra and inter-molecular energy versus time. a) The average incident particles velocities are $V_i = 3$ km.s$^{-1}$. b) The average incident particles velocities are $V_i = 9$ km.s$^{-1}$.

Thereafter, if the contribution of energy is more important, the energy brings by the incident particles can diffuse to other polymer chains by the intermediary of inter-molecular potentials, Lennard-Jones ($V_{vdw}$) and electrostatic forces ($V_{elec}$). This kind of energy transfer is less efficient than the intra-molecular, it is the reason for which, in Figure 3.b, the inter-molecular potential has the weakest variation of the polymer total energy, less of 5%.

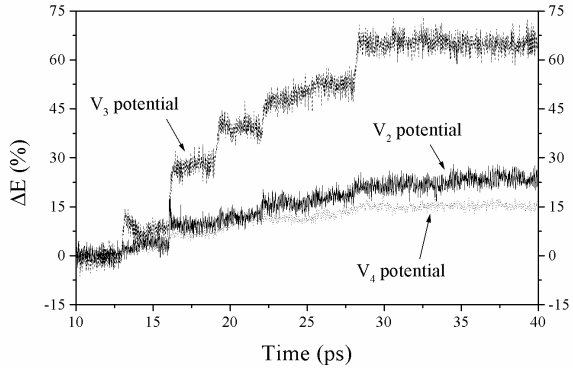


Fig. 4. Time evolution of the polyethylene crystal intra-molecular potentials: the average incident particles velocities are $V_i = 9$ km.s$^{-1}$.

### 3.3 Radius of gyration

The radius of gyration can be used to describe the orientation changes of the polyethylene chains. The radius of gyration ($R_g$) and its three Cartesian components ($R_{gx}$, $R_{gy}$ and $R_{gz}$) are given by [17]:

$$R_g^2 = \frac{1}{n}\sum_{i=1}^{n}\left\langle \left(\mathbf{r}_i - \mathbf{r}_c\right)^2 \right\rangle \tag{13}$$

$$\begin{cases} R_{gx}^2 = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n}\left\langle \left(\mathrm{x}_i - \mathrm{x}_c\right)^2 \right\rangle \\ R_{gy}^2 = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n}\left\langle \left(\mathrm{y}_i - \mathrm{y}_c\right)^2 \right\rangle \\ R_{gz}^2 = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n}\left\langle \left(\mathrm{z}_i - \mathrm{z}_c\right)^2 \right\rangle \end{cases} \tag{14}$$

where $\mathbf{r}_i = \left(x_i, y_i, z_i\right)$ is the position vector of the $i$th carbon atom, $\mathbf{r}_c = \left(x_c, y_c, z_c\right)$ the position vector of the center of mass of the $i$th chain. $x_i$, $y_i$, $z_i$ and $x_c$, $y_c$ , $z_c$ are the Cartesian coordinates of the $i$th atom, and of the center of mass of the $i$th chain, respectively. $\langle\cdots\rangle$ denotes the ensemble average, thus we have:

$$R_g^2 = R_{gx}^2 + R_{gy}^2 + R_{gz}^2 \tag{15}$$

The radius of gyration of the polyethylene crystal versus timestep for the two average incident particles velocities $V_i = 3$ and 9 km.s$^{-1}$ is given in Figure 5. For the incident particle velocity of 3 km.s$^{-1}$, the curve is regular and

shows that there is no particular evolution of the radius of gyration of the polyethylene crystal versus timestep. It is in a good agreement with our previous discussion, the interaction is weak and the energy brings by the incident particles is not enough important to drag some defects in the molecular structure of the polymer. For the other average velocity shown in Figure 5, we can see that, approximately, in the middle time of the simulation, there is a slight variation of the radius of gyration. Although this variation is not meaningful to give a conclusion, the contribution of energy of the incident particles is now sufficient to disturb the molecular arrangement of the polymer. It could be interesting to value the radius of gyration in several local parts of the polymer and to compare the results. This kind of calculations could underline a hypothetical local change of state of the polyethylene crystal maybe.

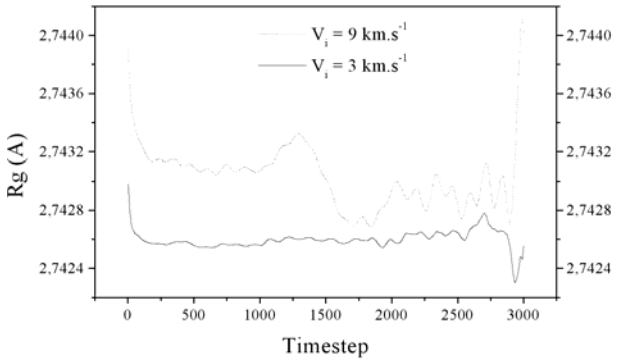


Fig. 5. Radius of gyration of the polyethylene crystal versus timestep: the average incident particles velocities are $V_i$ = 3 and 9 km.s$^{-1}$.

## 4. CONCLUSIONS

In application of industrial devices, we have performed molecular dynamic simulations to understand the process of the deterioration of the material. For this, several different particles, the $SF_6$ molecules and the copper ions, have impacted the polymer area, with an average incident velocity that varies from 3, 5, 7 to 9 km.s$^{-1}$. We have shown that for the lowest speed, the interaction has been too weak to conclude. Concerning the other cases, we have differentiated intra and inter-molecular potentials, used in the model, to give some explanations about the molecular disorder inside the polymer. We have presented that the energy of the incident particles has essentially been dissipated by intra-molecular potential, especially by the $V_3$ potential, due to the boundary condition along Oz axis. In the case where the average velocities of the incident particles have been the biggest, the interaction has been the strongest with a meaningful increase of the crystal temperature. But, when we have calculated the radius of gyration of the crystal, that was a good parameter to probe the molecular disorder in the crystal, we have not observed a significant evolution to be sure that there has been enough energy to induce a change of state of the material. In fact, we began to observe small defects in the polyethylene crystal with the bigger average speed of the incident particles. These results are in a good agreement with our previous works [12,18], where we have shown that an important particle velocity is needed to observe some damages of the target with disrupting chemical bonds.

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